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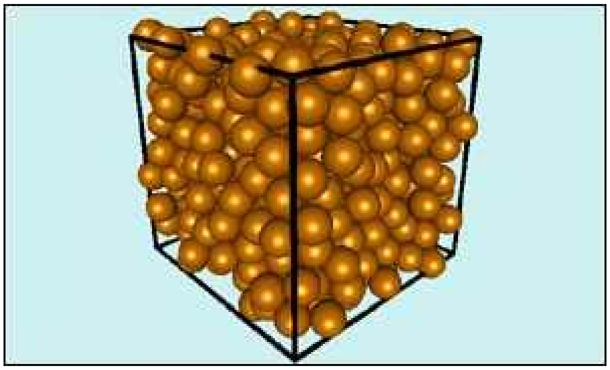
Unpacking a particle problem



The problem interests materials scientists

US researchers have put forward a new view on a problem that has fascinated mathematicians since biblical times.

It concerns what is sometimes called "particle packing" - how spheres, whether oranges or molecules, stack up when poured randomly into a vessel.

Understanding exactly how the particles in a system fall into place has important implications for many fields of science. Materials scientists are particularly interested in the subject.

Some of the newest materials are engineered on a scale that can be measured in billionths of a metre - nanometres. These materials have unusual electrical and optical properties because of the very precise way in which their atoms are arranged. Finding new ways of "pushing" atoms and molecules into particular arrangements has therefore become an important goal.

Experiments have even been done on the space shuttle to study how packing might be influenced in a micro-gravity environment.

Stirring and shaking

Researchers looking at the problem of stacking have long accepted the notion that, given enough stirring and shaking, a random collection of particles will always settle to a maximum density, a state known as random close packing.

Particles in that state were believed always to have the same density - about 64%. For example, if you poured marbles into a box, they would always pack so that they occupy

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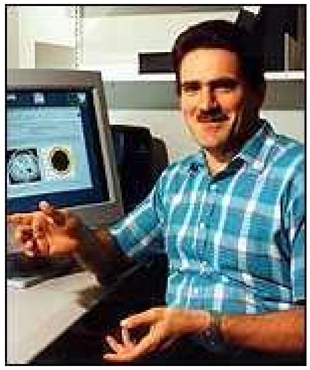
64% of the space and the rest is open air.


Sal Torquato: "The concept was totally ill-defined."

But Sal Torquato, Professor of Chemistry at Princeton University, argues that the concept of random close packing is deeply flawed and that the 64% figure is not at all universal.

Torquato and his colleagues used a combination of computer simulations and theoretical observations. They showed that the density of a randomly packed structure depends in large part on how the shaking, stirring and pouring is done.

That is, the marbles may fit perfectly into a container if they are poured one way, but may not fit if they are poured another way. That observation, says Professor Torquato, negates the idea that there is a fixed concept called random close packing.

Packing strategy

"People have been trying for years to theoretically predict what the percentage would be - to no avail," says Professor Torquato. "And it's because the concept was totally ill-defined."

Scholars have been interested in how particles pack together since antiquity, when a fair system of taxation or commerce depended on knowing how much material could be expected to fill a particular container. There is even a reference to the problem in the bible.

Scientists have long known the most efficient way of putting spherical particles together when the packing is done in an ordered, non-random way.

The mathematician and astronomer Johannes Kepler first predicted that the best packing strategy would yield a density of about 74%. That figure, which was only recently proved in a formal way, is called the "face-centred cubic (fcc)" array. It corresponds to the crystalline form taken by the atoms in many metals such as gold.

But getting to grips with randomly packed particles is trickier.

Jammed state

A variety of experiments have yielded results between 60% and 68%. Professor Torquato and colleagues report that the same "random" method of packing can result in a range of densities all the way from 64% to 74%. The problem, says Professor Torquato, is that the concept of randomness is too vague.

"When people called it 'random close packing,' they had no idea what they meant by randomness." He adds: "The notion of 'randomness' conflicts with that of 'close-packing,' which implies the most ordered structure."

To resolve the problem, the Princeton team proposed a formal method for measuring randomness, a mathematical expression for how strongly the structure varies from the most ordered fcc array.

They then proposed an entirely different concept, called the maximally random jammed state. The idea is to look for any combination of particles that is so tightly packed that none of the particles can move - a jammed state - and then measure how much randomness the structure contains.

In their computer simulations, the most disordered structure wound up having a density of 64%.

The Princeton work is featured in the latest issue of Physical Review Letters.

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